Electronic Supplementary Information

Epitaxial growth of $ZrSe_2$ nanosheets on sapphire by chemical vapor deposition for optoelectronic application

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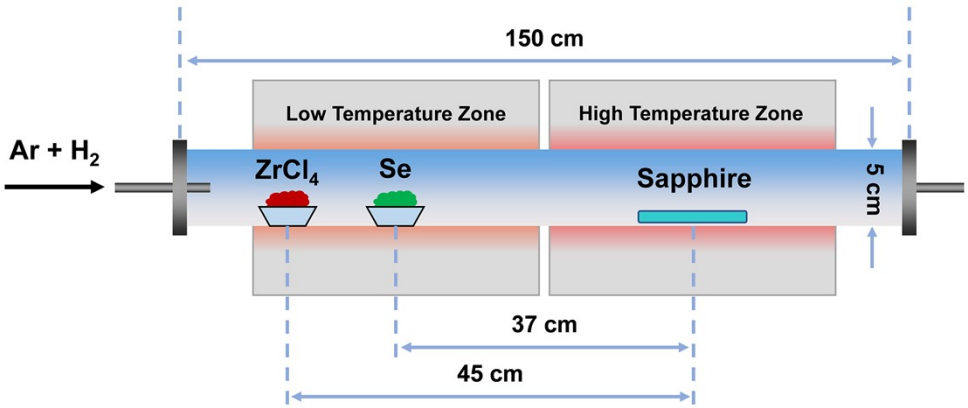

Figure S1. Schematic diagram of the CVD system with two independently controlled temperature zones for the epitaxial growth of $ZrSe_2$ layers. The diameter and length of the quartz tube and 5 cm and 150 cm, respectively. $ZrCl_4$ powder and sapphire substrates were put in the center of low-temperature (LT) and high-temperature (HT) zones, respectively. The Se and $ZrCl_4$ powders were typically placed at the upstream 37 cm and 45 cm away from the substrate, respectively.

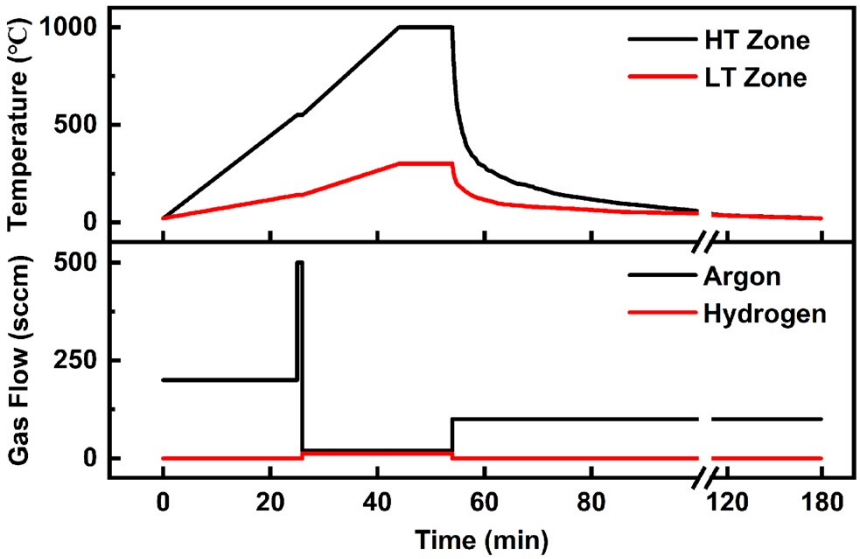

Figure S2. The temperature and the gas flow programming process used for a typical growth of $ZrSe_2$ layers by CVD. A burst of Ar flow for 2 min at 550 °C occurred to drive away premature excess $ZrCl_4$ vapor and prevent the over- or undersupply of Cl and Se.

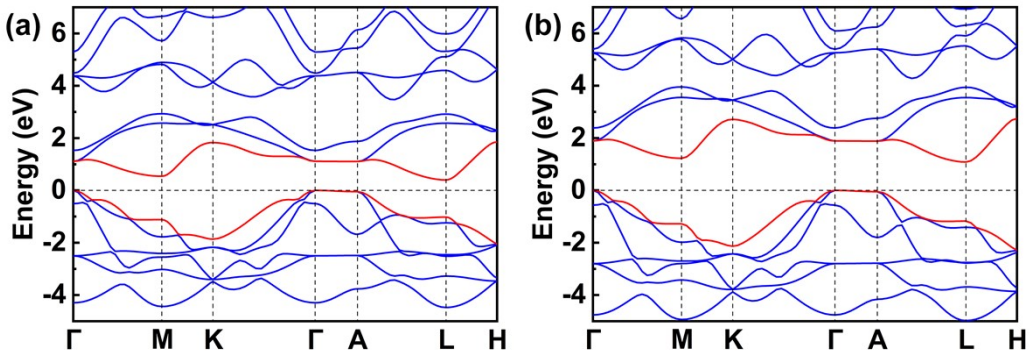

Figure S3. Electronic band structures of bulk 1T-$ZrSe_2$ with the theoretically optimized lattice constants on the relaxed structure ($a = b = 3.798$ Å, $c = 6.878$ Å) under d) PBE and e) HSE06. Red lines indicate the VBM and CBM.

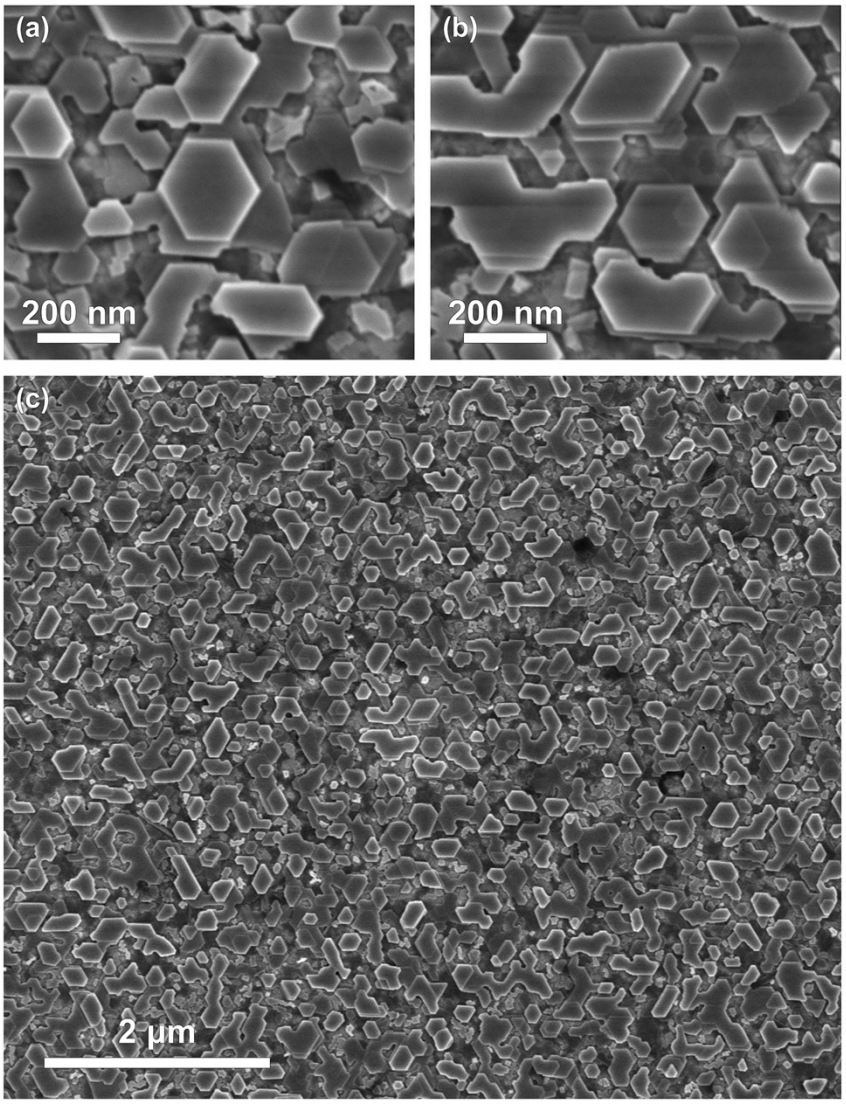

Figure S4. Typical SEM images with different magnifications of the CVD-grown $ZrSe_2$ nanosheets on sapphire substrate.

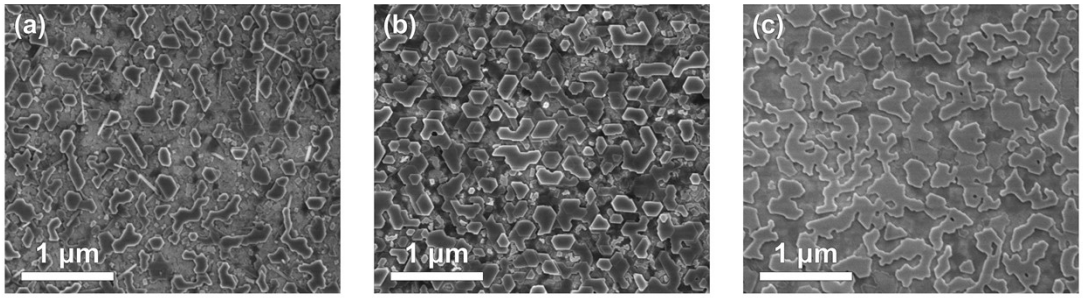

Figure S5. The SEM images of the $ZrSe_2$ nanosheets grown on sapphire substrates at different Se-source temperatures of a) 250, b) 300, c) 350 °C.

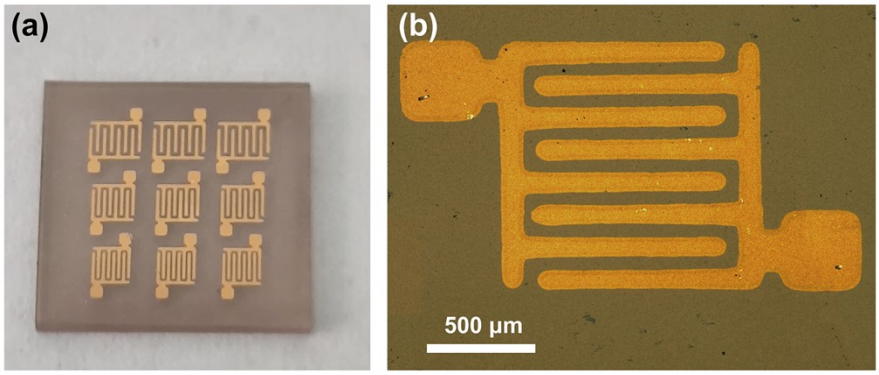

Figure S6. a) The photograph and b) optical micrograph of the $ZrSe_2$-based photodetector. The distance between two adjacent Au electrodes is estimated to be 70 µm.

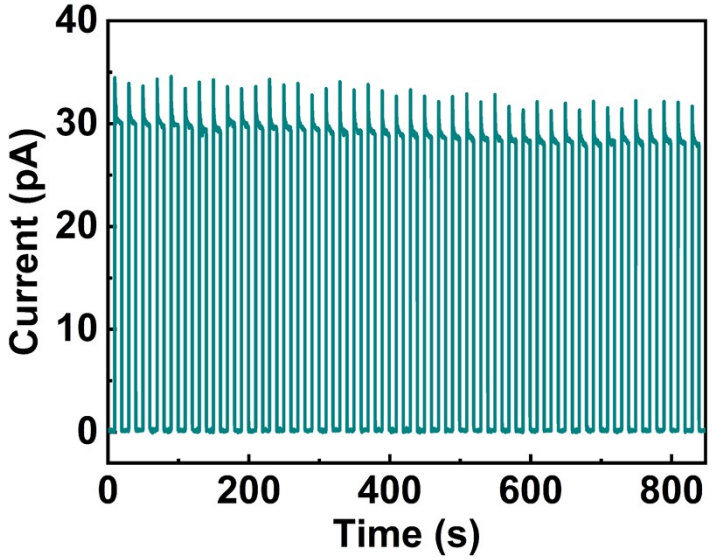

Figure S7. Operational stability of the $ZrSe_2$ photodetector measured at 10 V for 40 switching cycles.